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Multi-scale constitutive model for a wood-inspired composite

Saavedra Flores E. I. ^{*}, Murugan, M. S., Friswell, M. I., de Souza Neto E. A.

College of Engineering, Swansea University, Singleton Park, Swansea SA2 8PP, United Kingdom.

Abstract

This paper proposes a fully coupled multi-scale finite element model for the mechanical description of a new composite material inspired in wood cell-walls. The constitutive response of the composite is described by means of a representative volume element (RVE) in which the fibre is represented as a periodic alternation of rigid and soft portions of material. Furthermore, at a lower scale the overall constitutive behavior of the fibre is modelled as a single material defined by a second RVE. Numerical tests demonstrate substantial gains in terms of resistance to failure, toughness and in the control of the overall flexibility/stiffness balance in the material.

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1. Introduction

Wood microstructure can be understood as the result of an optimisation process developed by nature over millions of years. One of its main features is its hierarchical nature distributed across multiple spatial scales. This important feature has been widely investigated over the last few years by means of multi-scale finite element models in the context of elastic response [1-4], and recently in the context of irreversible behavior [5], bringing substantial progress to the understanding of this material.

In an attempt to exploit further the structural and mechanical concepts involved in wood cells, our main objective in this paper is to investigate the mechanical response of a new wood-inspired composite by means of a finite element-based computational multi-scale approach. Based on the wood cell-wall composite, the material response is described by means of a Representative Volume Element (RVE) composed of a biphasic fibre embedded in a soft matrix. Furthermore, at a lower scale the fibre is

^{*} Corresponding author. Tel.: + 44 (0) 1792 513177; fax: + 44 (0) 1792 295157.
E-mail address: e.i.saavedra-flores@swansea.ac.uk

represented as a periodic alternation of rigid and soft portions, whose overall constitutive behaviour is modelled as a single material defined at each Gauss-point by means of a second RVE. This bio-inspired strategy is suggested by the strong influence of the proportion of volume fractions of crystalline and amorphous celluloses on the overall mechanical behaviour of wood cells.

It is important to emphasise that the same periodic multi-scale framework has been adopted originally in [5] to investigate the wood cell-wall mechanics. In this paper however, we adopt this framework to study this new composite material.

The paper is organised as follows. Section 2 presents a brief review of wood cell-wall mechanics. The finite element-based multi-scale model of a wood-inspired composite and some numerical results are presented in Section 3. Finally, Section 4 summarises the main conclusions.

2. Wood cell-wall mechanics

The walls of wood cells contain three major chemical constituents: cellulose, hemicellulose and lignin. These constituents form a spatial arrangement called *microfibril* which can be represented as a periodic unit building block of rectangular cross-section with infinite length (see Figure 1(a)).

Cellulose, hemicellulose and lignin constitute approximately 30%, 30-35% and 35-40%, respectively, of the total volume of wood substance. The cellulose is a long polymer composed of glucose units which is organised into periodic crystalline and amorphous regions along its length and called crystalline-amorphous cellulose core as shown in Figure 1(b). This periodic arrangement is further covered with an outer surface made up of amorphous cellulose [6]. The (volumetric) degree of crystallinity is defined as the ratio between the volume of crystalline cellulose and the total volume of cellulose. Hemicellulose is a polymer with little strength built up of sugar units. Its structure is partially random with mechanical properties highly sensitive to moisture changes. Lignin is an amorphous polymer whose purpose is to cement the individual cells together and to provide shear strength. It is the most hydrophobic component in the cell-wall, with relatively stable mechanical properties under moisture changes. The specific orientation of *microfibrils* with respect to the longitudinal cell axis is called the *microfibril angle* (MFA) and is one of the most important parameters controlling the balance between stiffness and flexibility in trees.

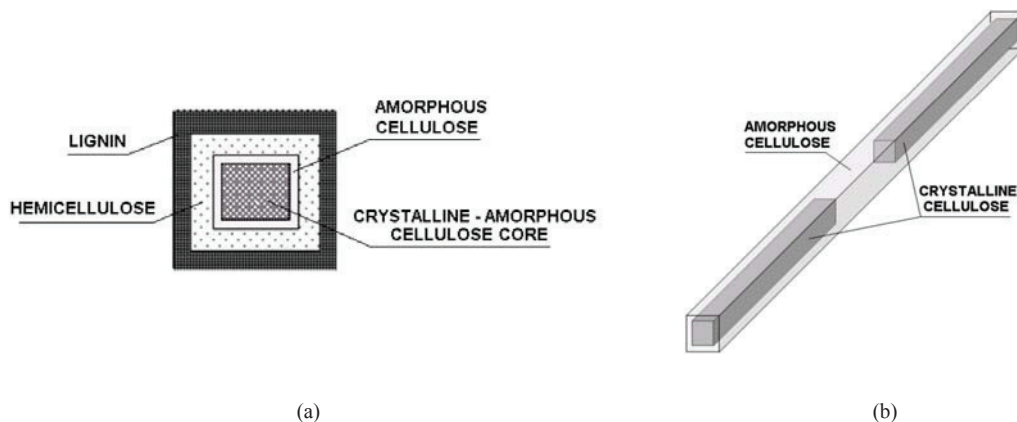


Fig. 1. (a) Representation of *microfibril* and basic constituents; (b) Representation of cellulose with its crystalline and amorphous fractions.

3. Multi-scale finite element model for a new wood-inspired composite

In this section we explore the design of a prototype wood-inspired composite when some of the structural and mechanical concepts involved in wood cells are exploited further. Based on the characteristics present in wood cell-walls, we suggest a bio-inspired strategy to increase the resistance to failure, toughness and to control the balance between stiffness and flexibility in a new composite.

In order to endow this composite with similar mechanisms of deformation found in the wood cell, we establish a one-to-one correspondence between each of the constituents present in wood and those existing in the new composite, and therefore the role performed by each of the cell-wall constituents is replicated in the new wood-inspired material. Thus, the reinforcing fibre of the new composite is assumed to be made up of two phases. The first phase is considered to be a very rigid elastic material (in the wood cell-wall composite, the stiff crystalline cellulose fibre), called here *RF* (Rigid portion of the Fibre). The second phase of the fibre is assumed to have a softer elasto-plastic response (the softer amorphous cellulose fraction in wood cell-wall), called *SF* (Softer fraction of the Fibre). Furthermore, the matrix is assumed to be formed by two phases, a very soft portion (in wood, the hemicellulose) called *SM* (Softer phase in the Matrix) and a relatively more rigid fraction (lignin in the cell-wall), called here *RM* (more Rigid fraction in the Matrix). Refer to Figure 2 for further details.

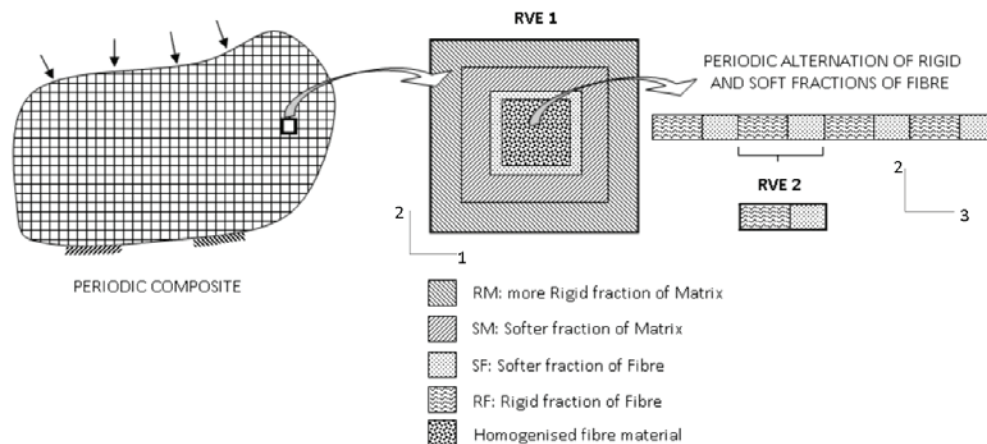


Fig. 2. Schematic representation of the wood-inspired composite and its constituents.

In order to mimic wood, we design this prototype with the same features found in wood. That is to say, we keep the same volume fractions of basic constituents. This means that we adopt a 30% volume fraction for the whole fibre, including *RF* and *SF*; and 32.5 and 37.5% for the two phases in the matrix, *SM* and *RM*, respectively. Similarly, we choose 52% for the percentage of volume of *RF* with respect to the entire volume of fibre (degree of crystallinity in the cellulose).

In this study, we adopt Alumina as the rigid elastic fraction of fibre, *RF*. Its mechanical properties are obtained from [7] and correspond to an isotropic material with Young's modulus $E=379$ GPa and Poisson's ratio $\nu=0.25$. Its tensile failure strain is 0.4%. To keep the same ratio present in the wood cell-wall composite, between the Young's modulus of the crystalline cellulose, $E=134$ GPa, and its amorphous counterpart, $E=10.42$ GPa, we proceed to define the Young's modulus of the softer fraction of fibre *SF* with a value $E=29.4715$ GPa, resulting in the same ratio $379/29.4715=134/10.42 = 12.86$. In order to endow this new composite with similar mechanisms of deformation found in the wood cell, we adopt the value of Poisson's ratio $\nu=0.23$ and failure strain $\varepsilon_f=0.03838$ (onset of plastic yielding) of the amorphous

cellulose fraction for the softer fraction of fibre SF in the new composite. With the above Young's modulus $E=29.4715$ GPa and failure strain $\varepsilon_f=0.03838$, we calculate a yield stress $\sigma_y=1.131$ GPa for SF .

For the definition of the mechanical properties of the matrix with its two phases, SM and RM , we follow the same considerations explained above. In addition, we adopt the same viscosity-related properties found in the hemicellulose and lignin for the softer and more rigid phases in the matrix, SM and RM , respectively (we refer to [5] for further details about the mechanical properties of the wood constituents). The resulting material constants for SM and RM along with those determined for RF and SF are summarised in Table 1.

Table 1. Summary of the mechanical properties adopted in the constituents of the present wood-inspired composite. The units for the Young's modulus E and yield stress σ_y are GPa. The units for the viscosity-related parameters η_p and η_m are GPa.s. Mechanical properties of Alumina are obtained from [7].

Constituents	E	ν	η_p	η_m	σ_y
RF (Alumina -- Rigid fraction of Fibre)	379	0.25	-	-	-
SF (Softer fraction of Fibre)	29.4715	0.23	-	-	1,131
SM (Softer fraction in Matrix)	0.1131	0.2	8.5	3.1	$5.37e-2$
RM (more Rigid fraction in Matrix)	4.4122	0.3	20.0	6.5	$5.37e-2$

The mechanical response of the composite is defined by a single material whose constitutive description is obtained by the computational homogenisation of the RVE 1 (*microfibril* scale), shown in Figure 2. Furthermore, at a lower scale the fibre is represented as a periodic alternation of rigid and soft portions, whose overall constitutive behaviour is modelled as a single material defined at each Gauss-point by means of the RVE 2 (refer to Figure 2).

We remark that the same multi-scale framework has been adopted in [5] to investigate the dissipative behavior of wood cell-walls. However, in this paper we adopt this framework to study this new composite material. Therefore, the finite element meshes for RVE 1 and 2 are obtained from [5].

The end strain state to be prescribed incrementally on the corresponding RVE 1 is calculated under the same assumptions made in [5, 8]. If the initial orientation of the fibre with respect to the y -direction (stretching axis) is 45° , then the in-plane Poisson's ratio can be estimated [5] as $\nu=[\cot(45^\circ)]^2=1$. Therefore, if the strain component applied in y -direction is 0.20, then the final strain state can be expressed as $\boldsymbol{\varepsilon}=\{-0.2,0.2,0,0,0,0\}^T$, in standard engineering strain array format.

In order to investigate the material response, we explore the influence of the volume fraction (V_f) of the constituent RF (with respect to the total volume of fibre) on the overall mechanical response of the new material. We compare the material response predicted for four different fractions: 0.45, 0.50, 0.55 and 0.60. Furthermore, we analyse the traditional condition in which the fibre is considered to be made of one single elastic material (in other words, $V_f=1.0$). The adopted strain rate is $1.25e-3$ s⁻¹.

Figure 3 shows the stress-strain curves for the different volume fractions V_f considered. In the corresponding graph, we see that for volume fractions V_f between 0.45 and 0.60 the mechanical response is virtually independent of V_f for strains under 4-5%. From the numerical results, it can be concluded that up to this level of strain, the whole fibre remains almost inextensible. After 8-9% of strain, however, the dependence of the response on the volume fraction V_f varies. When these curves ($V_f=0.45, 0.50, 0.55$ and 0.60) are compared to the condition $V_f=1$, the response becomes practically independent of V_f only for strains under 1.25%.

The small influence of V_f on the overall mechanical response at lower strain levels is attributed to the large angle (near 45°) between the fibre and the stretching axis at this stage. Here, only a small portion of

the axial load is carried by the fibre. In addition, the main mechanism of deformation in the composite is shear, localised in the matrix, due to the relative displacements among fibres undergoing rigid body rotation and alignment in the stretching direction. Therefore, any increase of the stiffness in the fibre due to a rise in the volume fraction of the stiff portion RF will not affect significantly the overall mechanical response of the composite under low strain levels since the fibre will experience predominantly changes in its orientation rather than straining along its own axis. If the straining process continues, the angle between the fibre and the stretching axis will reduce considerably and the fibres will begin to take larger portions of axial loads and the corresponding alignment will result in fibre reorientation-induced stiffening, as shown in Figure 3. Consequently, for only moderate to large strains the choice of different volume fractions V_f in the fibre will lead to different levels of stiffness in the material. On the contrary, for smaller strains (possible during service conditions) the amount of rigid fraction in the fibre will have virtually no influence on the overall response of the material.

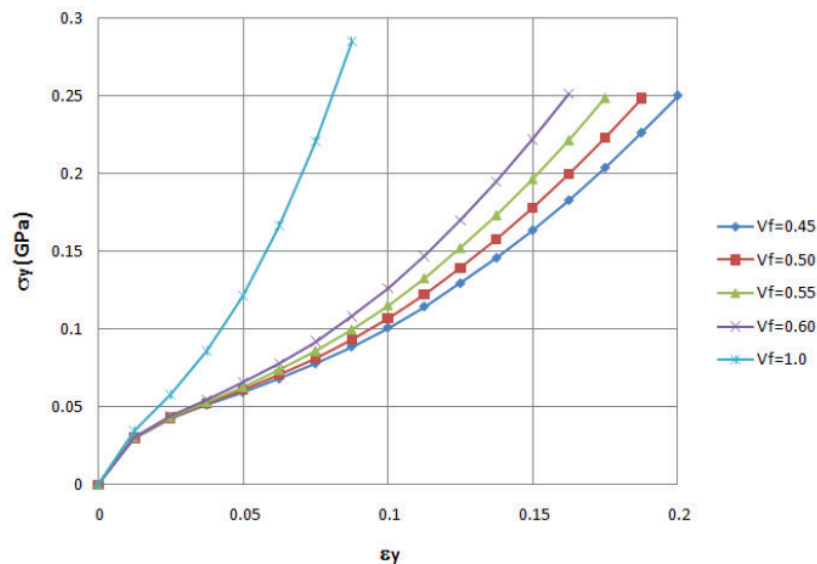


Fig. 3. Stress-strain diagrams in the wood-inspired composite, obtained from the RVE with different volume fractions V_f (volume of RF with respect to the whole volume of fibre).

Importantly, the curve shown in Figure 3 for $V_f=1$ has been truncated for a maximum strain of the (single material) fibre equal to 0.4% (the failure strain of Alumina [7]). Similarly, the remaining four curves for V_f between 0.45 and 0.60 have been truncated at failure. However, the mechanism of failure in this case is represented by the onset of plastic strain in the softer fraction of the fibre (SF) rather than failure in the rigid portion RF . This redistribution of the failure from the rigid constituent of the fibre to its softer counterpart allows the composite to increase substantially the strain to failure, from almost 9% (for the classical solution $V_f=1$) to 20% strain ($V_f=0.45$), without showing significant reduction in the maximum stress (just a drop from 0.285 to 0.25 GPa).

In addition, a quick examination of this graph shows that the area under the curve for the particular case of $V_f=0.45$ almost duplicates the area under the curve corresponding to $V_f=1$, indicating an increase in the toughness of the material when almost half of the original (single material) elastic fibre is replaced with a softer fraction.

It is important to note that in [8] it was shown how wood tissue and individual cells are able to undergo large deformations without apparent damage in the hemicellulose-lignin matrix. This process is

interpreted as a *stick-slip* mechanism at the molecular level of the matrix which results in a plastic response similar to crystallographic sliding in polycrystalline metals. Therefore, inspired in this feature, the proposed matrix in this composite does show plastic response but does not jeopardize the integrity of the entire unit. We also remark that the main mechanism of failure in the wood cell-wall under straining has been demonstrated to be the onset of inelastic yielding in the amorphous fraction of the cellulose fibre [5] which is consistent with the failure mechanism shown in this proposed wood-inspired composite material.

4. Conclusions

Fundamental concepts involved in wood cells mechanics have been exploited in order to design a new wood-inspired composite. A finite element-based computational multi-scale framework has been adopted to investigate the mechanical response of this new material. Numerical results have demonstrated substantial gains in terms of resistance to failure, toughness and in the control of the overall flexibility/stiffness balance in the material. We have shown here that the introduction of a very simple wood-inspired strategy allows the composite to increase substantially its strain to failure, from 9% (for the classical engineering solution considering a single material fibre) up to 20% strain (when almost half of the original elastic fibre is replaced with a softer fraction), without showing significant reduction in the maximum stress.

The features presented above have been replicated from wood and represent a natural mechanism of adaptation to the development of large strains in trees.

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